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NEWS
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                 Simultaneous left and right truncation (SLART) added
                 for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
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         FEB 02
                 GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS
         FEB 06
                 Patent sequence location (PSL) data added to USGENE
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         FEB 10
                 COMPENDEX reloaded and enhanced
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         FEB 11
                 WTEXTILES reloaded and enhanced
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         FEB 19
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NEWS 10
         FEB 23
                 Several formats for image display and print options
                 discontinued in USPATFULL and USPAT2
         FEB 23
                 MEDLINE now offers more precise author group fields
NEWS 11
                 and 2009 MeSH terms
         FEB 23
                 TOXCENTER updates mirror those of MEDLINE - more
NEWS 12
                 precise author group fields and 2009 MeSH terms
NEWS 13
         FEB 23
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                 STN patent clusters
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         FEB 25
                 USGENE enhanced with patent family and legal status
                 display data from INPADOCDB
NEWS 15
         MAR 06
                 INPADOCDB and INPAFAMDB enhanced with new display
                 formats
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         MAR 11
                 EPFULL backfile enhanced with additional full-text
                 applications and grants
NEWS 17
         MAR 11
                 ESBIOBASE reloaded and enhanced
                 CAS databases on STN enhanced with new super role
NEWS 18
         MAR 20
                 for nanomaterial substances
                 CA/CAplus enhanced with more than 250,000 patent
NEWS 19
         MAR 23
                 equivalents from China
NEWS 20
         MAR 30
                 IMSPATENTS reloaded and enhanced
NEWS 21
         APR 03
                 CAS coverage of exemplified prophetic substances
                  enhanced
NEWS 22
         APR 07
                 STN is raising the limits on saved answers
NEWS 23
         APR 24
                 CA/CAplus now has more comprehensive patent assignee
                  information
NEWS 24
         APR 26
                 USPATFULL and USPAT2 enhanced with patent
                  assignment/reassignment information
NEWS 25
         APR 28
                 CAS patent authority coverage expanded
NEWS 26
         APR 28
                 ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 27
         APR 28
                 Limits doubled for structure searching in CAS
                 REGISTRY
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NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

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STRUCTURE FILE UPDATES: 5 MAY 2009 HIGHEST RN 1143038-16-7 DICTIONARY FILE UPDATES: 5 MAY 2009 HIGHEST RN 1143038-16-7

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chain nodes :
21 22 23 24 25 27 29 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 26 28 30 31 32 33
34 35 36 37 38 39 40 41 42
ring/chain nodes :
18 20
chain bonds :
10-12 \quad 15-18 \quad 18-20 \quad 20-21 \quad 22-23 \quad 23-24 \quad 25-26 \quad 27-28 \quad 29-30 \quad 36-43 \quad 40-44
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-11 \quad 7-8 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14
14-15 15-16 16-17 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33 33-34
35-36 36-37 37-38 39-40 40-41 41-42
exact/norm bonds :
7-11 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33
33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42
exact bonds :
7-8 8-9 10-12 15-18 18-20 25-26 27-28 29-30
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-17 \quad 22-23
23-24
isolated ring systems :
containing 1:7:12:
```

G1:[*1],[*2],[*3],[*4]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom
29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS 50:Atom

L1STRUCTURE UPLOADED

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FULL SEARCH INITIATED 20:34:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -74 TO ITERATE

100.0% PROCESSED 74 ITERATIONS 37 ANSWERS

SEARCH TIME: 00.00.01

37 SEA SSS FUL L1 L2

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chain nodes :

21 22 23 24 25 27 29 43 44

ring nodes :

ring/chain nodes :

18 20

chain bonds :

 $5-7 \quad 10-12 \quad 15-18 \quad 18-20 \quad 20-21 \quad 22-23 \quad 23-24 \quad 25-26 \quad 27-28 \quad 29-30 \quad 36-43 \quad 40-44$

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14$

 $14 - 15 \quad 15 - 16 \quad 16 - 17 \quad 26 - 31 \quad 26 - 34 \quad 28 - 35 \quad 28 - 38 \quad 30 - 39 \quad 30 - 42 \quad 31 - 32 \quad 32 - 33 \quad 33 - 34 \quad 32 - 33 \quad 33 - 34 \quad 33 -$

35-36 36-37 37-38 39-40 40-41 41-42

exact/norm bonds:
7-11 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33 33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42 exact bonds:
5-7 7-8 8-9 10-12 15-18 18-20 25-26 27-28 29-30 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17 22-23 23-24 isolated ring systems:

isolated ring systems :
containing 1 : 7 : 12 :

G1:[*1],[*2],[*3],[*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom 29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS

L3 STRUCTURE UPLOADED

=> s 13 sss full FULL SEARCH INITIATED 20:34:48 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 224 TO ITERATE

100.0% PROCESSED 224 ITERATIONS 38 ANSWERS

SEARCH TIME: 00.00.01

L4 38 SEA SSS FUL L3

=> file capl

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
371.76
371.98

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FILE LAST UPDATED: 5 May 2009 (20090505/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC)

reclassification data for the third quarter of 2008.

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6 L2

=> s 14

L6 5 L4

=> s 15 or 16

L7 8 L5 OR L6

=> d 17 1-8 ibib hitstr

L7 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:1158632 CAPLUS

DOCUMENT NUMBER: 149:402366

TITLE: Preparation of aminopyridine derivatives, particularly

3-(aminopyridinyl)-5-(alkoxyphenyl)-1,2,4-oxadiazoles,

as immunomodulating S1P1/EDG1 receptor agonists

INVENTOR(S): Bolli, Martin; Mathys, Boris; Mueller, Claus; Nayler,

Oliver; Steiner, Beat; Velker, Joerg

APPLICATION NO.

DATE

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd, Switz.

KIND DATE

SOURCE: PCT Int. Appl., 121pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

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WO	2008	${1141}$	 57		A1		2008	 0925							2	0080	229
	W:	ΑE,	ΑG,	AL,	AM,	AO,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,
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		FΙ,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,
		KG,	KM,	KN,	KP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,
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	hylp	_		_					_				_	_	opio	nic	acid
106	2670	-96-	5P,	3 – [4	-[5-	(2-D	ieth	ylam	ino-	6-me	thyl	pyri	din-	4-			
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RN 1062670-28-3 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-[methyl(1-methylethyl)amino]-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 1062670-96-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[2-(diethylamino)-6-methyl-4-pyridinyl]-1,2,4-oxadiazol-3-yl]-2-ethyl-6-methyl- (CA INDEX NAME)

IT 1062673-09-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of aminopyridine derivs. as immunomodulating S1P1/EDG1 receptor agonists)

RN 1062673-09-9 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-[(1-methylethyl)amino]-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

IT 1062669-77-5P, 3-[2-Ethyl-4-[5-[2-[(ethyl)(methyl)amino]-6methylpyridin-4-yl][1,2,4]oxadiazol-3-yl]-6-methylphenyl]propionic acid
RL: SPN (Synthetic preparation); PREP (Preparation)

(drug candidate; preparation of aminopyridine derivs. as immunomodulating ${\tt S1P1/EDG1}$ receptor agonists)

RN 1062669-77-5 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-4-[5-[2-(ethylmethylamino)-6-methyl-4-pyridinyl]-1,2,4-oxadiazol-3-yl]-6-methyl- (CA INDEX NAME)

IT 1062673-25-9P, 3-[2-Ethyl-6-methyl-4-[5-[2-methyl-6-(morpholin-4-yl)pyridin-4-yl][1,2,4]oxadiazol-3-yl]phenyl]propionic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminopyridine derivs. as immunomodulating S1P1/EDG1 receptor agonists)

RN 1062673-25-9 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-(4-morpholinyl)-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:411236 CAPLUS

DOCUMENT NUMBER: 148:403230

TITLE: Preparation of diaryloxadiazole derivatives for use as

antiinflammatory and immunosuppressive agents
INVENTOR(S): Albert, Rainer; Cooke, Nigel Graham; Lewis, Ian;

Weiler, Sven; Zecri, Frederic

PATENT ASSIGNEE(S): Novartis A.-G., Switz. SOURCE: PCT Int. Appl., 35pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT N	KIN	D	DATE		1	APPL	ICAT		DATE							
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WO 2008037476			A1		2008	0403	1	WO 2	007-:		20070927					
W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,
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	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,
	KM,	KN,	KP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	ME,
	MG,	MK,	MN,	MW,	MX,	MY,	MΖ,	NA,	NG,	ΝΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,
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	IS,	ΙΤ,	LT,	LU,	LV,	MC,	MT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,
	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	ΤG,	BW,

GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,

BY, KG, KZ, MD, RU, TJ, TM

AU 2007302262 A1 20080403 AU 2007-302262 20070927 PRIORITY APPLN. INFO.: EP 2006-121495 A 20060929 WO 2007-EP8431 W 20070927

OTHER SOURCE(S): MARPAT 148:403230

IT 1016261-25-8P 1016261-26-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryloxadiazole derivs. for use as antiinflammatory and immunosuppressive agents)

RN 1016261-25-8 CAPLUS

CN L-Phenylalanine, 4-[5-[2-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 1016261-26-9 CAPLUS

CN D-Phenylalanine, 4-[5-[2-(trifluoromethyl)[1,1'-biphenyl]-4-yl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:322210 CAPLUS

DOCUMENT NUMBER: 148:355634

TITLE: Pyridin-3-yl derivatives as immunomodulating agents

and their preparation, pharmaceutical compositions and

use in the treatment of immune system disorders

INVENTOR(S): Bolli, Martin; Lehmann, David; Mathys, Boris; Mueller,

Claus; Nayler, Oliver; Steiner, Beat; Velker, Joerg

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.

SOURCE: PCT Int. Appl., 82pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PAT	NO.		KIN	D	DATE			APPL	ICAT	DATE							
WO 2008029370						_	2008	0313		 WO 2	 007-		20070906				
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BH,	BR,	BW,	BY,	BZ,	CA,
		CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	FI,
		GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,
		KM,	KN,	KP,	KR,	KΖ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	ΜE,
		MG,	MK,	MN,	MW,	MX,	MY,	MΖ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,
		PT,	RO,	RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ΤJ,	TM,	TN,
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		ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,
		GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,
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PRIORITY APPLN. INFO.:

WO 2006-IB53187 A 20060908

OTHER SOURCE(S): MARPAT 148:355634

1011476-25-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate and intermediate; preparation of pyridinyl derivs. as immunomodulating agents useful in the treatment of immune system disorders)

1011476-25-7 CAPLUS RN

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[5-methyl-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

i-Pro N
$$\operatorname{CH}_2-\operatorname{CH}_2-\operatorname{CO}_2\operatorname{H}$$

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:322202 CAPLUS

DOCUMENT NUMBER: 148:331565

TITLE: Pyridin-4-yl derivatives as immunomodulating agents

and their preparation, pharmaceutical compositions and

use in the treatment of immune system disorders Bolli, Martin; Lehmann, David; Mathys, Boris; Mueller, INVENTOR(S):

Claus; Nayler, Oliver; Steiner, Beat; Velker, Joerg

PATENT ASSIGNEE(S): Actelion Pharmaceuticals Ltd., Switz.

SOURCE: PCT Int. Appl., 132pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE _____

WO 2008029371 20080313 WO 2007-IB53594 20070906 Α1 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, W: CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:

WO 2006-IB53147 A 20060907

OTHER SOURCE(S):

MARPAT 148:331565

IT 1011264-28-0P 1011264-30-4P 1011264-32-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of pyridinyl derivs. as immunomodulating agents useful in the treatment of immune system disorders)

RN 1011264-28-0 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-4-[5-(2-ethyl-6-methyl-4-pyridinyl)-1,2,4-oxadiazol-3-yl]-6-methyl- (CA INDEX NAME)

RN 1011264-30-4 CAPLUS

CN Benzenepropanoic acid, 2-ethyl-6-methyl-4-[5-[2-methyl-6-(2-methylpropyl)-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

i-Bu Et
$$\mathrm{CH}_2\mathrm{-CH}_2\mathrm{-CO}_2\mathrm{H}$$
 Me

RN 1011264-32-6 CAPLUS

CN Benzenepropanoic acid, 2,6-dimethyl-4-[5-[2-methyl-6-(2-methylpropyl)-4-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

i-Bu Me
$$CH_2-CH_2-CO_2H$$
 Me Me

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:81270 CAPLUS

DOCUMENT NUMBER: 146:337810

TITLE: SAR studies of 3-arylpropionic acids as potent and

selective agonists of sphingosine-1-phosphate receptor-1 (S1P1) with enhanced pharmacokinetic

properties

AUTHOR(S): Yan, Lin; Huo, Pei; Hale, Jeffrey J.; Mills, Sander

G.; Hajdu, Richard; Keohane, Carol A.; Rosenbach, Mark J.; Milligan, James A.; Shei, Gan-Ju; Chrebet, Gary; Bergstrom, James; Card, Deborah; Mandala, Suzanne M. Department of Medicinal Chemistry, Merck Research

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research

Laboratories, Rahway, NJ, 07065, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2007),

17(3), 828-831

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:337810

IT 856166-23-9P 856166-26-2P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP

(Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP

(Preparation)

(preparation, sphingosinephosphate receptor agonistic activity,

pharmacokinetics, and structure-activity relationship of

(oxadiazolylaryl)propionic acids using Heck coupling reaction)

RN 856166-23-9 CAPLUS

CN Benzenepropanoic acid, α , 3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 856166-26-2 CAPLUS

CN Benzenepropanoic acid, β , 3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1, 2, 4-oxadiazol-3-yl]- (CA INDEX NAME)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:548763 CAPLUS

DOCUMENT NUMBER: 145:180190

TITLE: Highly selective and potent agonists of

sphingosine-1-phosphate 1 (S1P1) receptor

AUTHOR(S): Vachal, Petr; Toth, Leslie M.; Hale, Jeffrey J.; Yan,

Lin; Mills, Sander G.; Chrebet, Gary L.; Koehane,

Carol A.; Hajdu, Richard; Milligan, James A.;

Rosenbach, Mark J.; Mandala, Suzanne

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck & Co., Inc.,

Rahway, NJ, 07065, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(14), 3684-3687

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

IT 856166-11-5P 856166-29-5P 856167-04-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(agonists of sphingosine-1-phosphate 1 receptor)

RN 856166-11-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} \\ \\ \text{i-PrO} \\ \\ \text{C1} \end{array}$$

RN 856166-29-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \end{array}$$

RN 856167-04-9 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \\ \hline \\ \text{CF}_3 \end{array}$$

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:548762 CAPLUS

DOCUMENT NUMBER: 145:210970

TITLE: Discovery of 3-arylpropionic acids as potent agonists

of sphingosine-1-phosphate receptor-1 (S1P1) with high

selectivity against all other known S1P receptor

subtypes

AUTHOR(S): Yan, Lin; Huo, Pei; Doherty, George; Toth, Lesile;

Hale, Jeffrey J.; Mills, Sander G.; Hajdu, Richard; Keohane, Carol A.; Rosenbach, Mark J.; Milligan, James A.; Shei, Gan-Ju; Chrebet, Gary; Bergstrom, James;

Card, Deborah; Quackenbush, Elizabeth; Wickham,

Alexandra; Mandala, Suzanne M.

CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research

Laboratories, Rahway, NJ, 07065, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(14), 3679-3683

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:210970 IT 856166-09-1P 856166-11-5P 856166-12-6P

856166-13-7P 856166-14-8P 856166-15-9P 856166-16-0P 856166-29-5P 856166-34-2P

856166-74-0P 856166-82-0P 856166-88-6P

856166-89-7P 856166-90-0P 856167-04-9P 905308-11-4P 905308-18-1P 905308-20-5P

905308-11-4P 905308-18-1P 905308-20-5P 905308-32-9P 905308-36-3P 905308-38-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(discovery of 3-arylpropionic acids as potent agonists of sphingosine-1-phosphate receptor-1 (S1P1) with high selectivity against

all other known S1P receptor subtypes)

RN 856166-09-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \end{array}$$

RN 856166-11-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{i-PrO} \\ \hline \\ \text{Cl} \end{array}$$

RN 856166-12-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-bromo-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CO}_2\text{H} \\ \\ \text{i-PrO} \\ \\ \text{Br} \end{array}$$

RN 856166-13-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-methoxy-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-14-8 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \end{array}$$

RN 856166-15-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-fluoro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \end{array}$$

RN 856166-16-0 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[5-(2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CO}_2\text{H} \\ \hline \\ \text{i--Bu} \\ \end{array}$$

RN 856166-29-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-CH_2-CO_2H \\ \hline \\ i-PrO \\ \hline \\ C1 \end{array}$$

RN 856166-34-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-74-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-(1,1-difluoro-2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$i-Pr-CF_2$$
 N
 $O-N$
 Me
 $CH_2-CH_2-CO_2H$

RN 856166-82-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-88-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{CN} & \operatorname{CN} \\ \operatorname{HO_2C-CH_2-CH_2} & \operatorname{O-CH_2-CF_3} \\ & \operatorname{N-O} \end{array}$$

RN 856166-89-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} \\ \\ \text{CF}_3 \\ \\ \text{CN} \end{array}$$

RN 856166-90-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[(1S)-1-methylpropoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 856167-04-9 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{i-PrO} \\ \\ \text{CF}_3 \end{array}$$

RN 905308-11-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-(4-cyclohexylphenyl)-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 905308-18-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-ethoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 905308-20-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-methoxy-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 905308-32-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-(5-butyl-2-pyridinyl)-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 905308-36-3 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[6-(2-methylpropyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 905308-38-5 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \\ \text{i-PrO} \end{array}$$

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:564648 CAPLUS

DOCUMENT NUMBER: 143:97368

TITLE: Preparation of five-membered heterocycle-substituted

benzenepropanoic and related acids as selective S1P1

(EDG1) receptor agonists

INVENTOR(S): Colandrea, Vincent J.; Doherty, George A.; Hale,

Jeffrey J.; Huo, Pei; Legiec, Irene E.; Toth, Leslie;

Vachal, Petr; Yan, Lin

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 230 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PAT	CENT	ΝΟ.			KIN	D	DATE			APPL	ICAT		DATE							
	WO	O 2005058848						2005	0630		WO 2	004-		20041213							
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,			
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,			
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,			
			LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	ΝI,			
			NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,			
			ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
		RW:	BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,			
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,			
			EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	IE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,			
			RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,			
			MR,	NE,	SN,	TD,	ΤG														
	AU 2004299456					Α1						004-									
	CA 2547198				A1		2005	0630		CA 2	004-		2	0041	213						
	EP 1697333				A1		2006	0906		EP 2	004-	8141	11		2	0041	213				
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,			
				SI,	LT,	•			•	•		CZ,	•		•						
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	met	hylp	heny	l]pr	opan	oic	acid	856	166-	12-6	Ρ,										

3-[4-[5-(4-Isopropoxy-3-bromophenyl)-1,2,4-oxadiazol-3-yl]-3-

3-[4-[5-(4-Isopropoxy-3-methoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-

methylphenyl]propanoic acid 856166-13-7P,

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methylphenyl]propanoic acid 856166-14-8P,
3-[4-[5-(4-Isopropoxy-3-methylphenyl)-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-15-9P,
3-[4-[5-(4-Isopropoxy-3-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-16-0P,
3-[4-[5-[5-(2-Methylpropyl)pyridin-2-y1]-1,2,4-oxadiazol-3-y1]-3-
methylphenyl]propanoic acid 856166-23-9P,
2-Methyl-3-[4-[5-[3-(trifluoromethyl)-4-isopropoxyphenyl]-1,2,4-oxadiazol-
3-yl]-3-methylphenyl]propanoic acid 856166-24-0P,
2-Methyl-3-[4-[5-(3-cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-25-1P,
2-Methyl-3-[4-[5-(3-methyl-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-26-2P,
3-[4-[5-[3-(Trifluoromethyl)-4-isopropoxyphenyl]-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]butanoic acid 856166-27-3P,
3-[4-[5-(3-Cyano-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]butanoic acid 856166-28-4P,
3-[4-[5-(3-Methyl-4-isopropoxyphenyl)-1, 2, 4-oxadiazol-3-yl]-3-
methylphenyl]butanoic acid 856166-29-5P,
3-[4-[5-(5-Chloro-6-isopropoxypyridin-3-y1)-1,2,4-oxadiazol-3-y1]-3-
methylphenyl]propanoic acid 856166-32-0P,
3-[4-[5-(5-Chloro-6-isopropylaminopyridin-3-y1)-1,2,4-oxadiazol-3-y1]-3-
methylphenyl]propanoic acid 856166-34-2P,
3-[4-[5-[5-Chloro-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-35-3P,
3-[4-[5-[5-Chloro-6-(pyrrolidin-1-yl)pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-36-4P,
3-[4-[5-[5-Chloro-6-(morpholin-4-yl)pyridin-3-yl]-1, 2, 4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-37-5P,
3-[4-[5-[5-Chloro-6-[(isopropyl)(methyl)amino]pyridin-3-yl]-1,2,4-
oxadiazol-3-y1]-3-methylphenyl]propanoic acid 856166-38-6P,
3-[4-[5-[5-Chloro-6-(2,2,2-trifluoroethoxy)]]-1,2,4-oxadiazol-3-
yl]-3-methylphenyl]butanoic acid 856166-39-7P,
3-[4-[5-[5-Chloro-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-40-0P,
3-[4-[5-[5-Chloro-6-(3,3-difluoropiperidin-1-yl)pyridin-3-yl]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-41-1P,
3-[4-[5-[5-Chloro-6-(3,3-difluoropyrrolidin-1-yl)pyridin-3-yl]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-42-2P,
3-[4-[5-[5-Trifluoromethyl-6-(morpholin-4-yl)pyridin-3-yl]-1,2,4-oxadiazol-
3-y1]-3-methylphenyl]butanoic acid 856166-48-8P,
3-[4-[5-(5-Chloro-6-isobutylpyridin-3-yl)-1,2,4-oxadiazol-3-yl]-3-
methylphenyl]propanoic acid 856166-50-2P,
3-[4-[5-[5-Iodo-6-(N-isopropyl-N-methylamino)pyridin-3-y1]-1,2,4-oxadiazol-
3-y1]-3-methylphenyl]propanoic acid 856166-51-3P,
oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-54-6P,
3-[4-[5-[6-(3,3-Difluoropyrrolidin-1-y1)-5-iodopyridin-3-y1]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-55-7P,
3-[4-[5-[6-(3,3-Difluoropyrrolidin-1-y1)-5-ethynylpyridin-3-y1]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-74-0P,
3-[4-[5-[5-(1,1-Difluoro-2-methylpropyl)pyridin-2-yl]-1,2,4-oxadiazol-3-
yl]-3-methylphenyl]propanoic acid 856166-75-1P,
3-[4-[5-(5-Cyano-6-ethoxypyridin-3-y1)-1,2,4-oxadiazol-3-y1]-3-
methylphenyl]propanoic acid 856166-76-2P,
3-[4-[5-[5-Cyano-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-
oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-77-3P,
methylphenyl]propanoic acid 856166-78-4P,
3-[4-[5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-[5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-[4-(5-[4-(1,1-Difluoro-2-methylpropyl)phenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenylphenyl
methylphenyl]propanoic acid 856166-79-5P,
3-[4-[5-[5-Iodo-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-oxadiazol-
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3-y1]-3-methylphenyl]propanoic acid 856166-80-8P, 3-[4-[5-[3-Chloro-4-(cyclopentyloxy)phenyl]-1,2,4-oxadiazol-3-yl]-3methylphenyl]propanoic acid 856166-81-9P, methylphenyl]propanoic acid 856166-82-0P, 3-[4-[5-[3-Cyano-4-[1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3yl]-3-methylphenyl]propanoic acid 856166-83-1P, 3-[4-[5-[3-Chloro-4-[1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3v1]-3-methylphenyl]propanoic acid 856166-84-2P, 3-[4-[5-(3,5-Dichloro-4-isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3methylphenyl]propanoic acid 856166-85-3P, 3-[4-[5-[3-Chloro-4-(cyclopropylmethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3methylphenyl]propanoic acid 856166-86-4P 856166-87-5P, 3-[4-[5-[3-Nitro-4-[1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3yl]-3-methylphenyl]propanoic acid 856166-88-6P, methylphenyl]propanoic acid 856166-89-7P, 3-[4-[5-[3-Cyano-4-[1-(trifluoromethyl)-2,2,2-trifluoroethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-90-0P yl]-3-methylphenyl]propanoic acid 856166-91-1P, 3-[4-[5-[4-(Trifluoromethyl)-6-[1-(trifluoromethyl)ethoxy]pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-92-2P 3-[4-[5-[4-Amino-6-(2,2,2-trifluoro-1-methylethoxy)]]-1,2,4oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856166-94-4P, 3-[4-[5-[3-Cyano-4-[((S)-1-methylpropyl)oxy]phenyl]-1, 2, 4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-95-5P, 3-[4-[5-[3-Cyano-4-[1-(trifluoromethyl)-2,2,2-trifluoroethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]butanoic acid 856166-96-6P, 3-[4-[5-[3-Cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3methylphenyl]butanoic acid 856167-09-4P 856167-14-1P 856167-19-6P, erythro-(±)-2,3-Dihydroxy-3-[4-[5-(3-cyano-4isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid 856167-21-0P, threo-(±)-2,3-Dihydroxy-3-[4-[5-(3-cyano-4isopropoxyphenyl)-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid oxadiazol-3-yl]-3-methylphenyl]propanoic acid RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of five-membered heterocycle-substituted benzenepropanoic and related acids as selective S1P1 (EDG1) receptor agonists) 856166-09-1 CAPLUS

RN

Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-CN oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} \\ \\ \text{i-PrO} \\ \\ \text{CN} \end{array}$$

RN 856166-11-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(1-methylethoxy)phenyl]-1,2,4oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{i-Pro} \\ \hline \\ \text{Cl} \end{array}$$

RN 856166-12-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-bromo-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \end{array}$$

RN 856166-13-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-methoxy-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{i-PrO} \\ \hline \\ \text{OMe} \end{array}$$

RN 856166-14-8 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \end{array}$$

RN 856166-15-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-fluoro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{i-PrO} \\ \hline \\ \text{F} \end{array}$$

RN 856166-16-0 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[5-(2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 856166-23-9 CAPLUS

CN Benzenepropanoic acid, α , 3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{CH}_2\text{-CH-CO}_2\text{H} \\ \\ \text{i-PrO} & \text{Me} \\ \\ & \text{CF}_3 \end{array}$$

RN 856166-24-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- α ,3-dimethyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{CH}_2\text{-}\text{CH-CO}_2\text{H} \\ \\ \text{i-PrO} & \text{Me} \\ \\ \text{CN} & \end{array}$$

RN 856166-25-1 CAPLUS

CN Benzenepropanoic acid, α , 3-dimethyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1, 2, 4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 856166-26-2 CAPLUS

CN Benzenepropanoic acid, β , 3-dimethyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{CH-CH}_2\text{-CO}_2\text{H} \\ \\ \text{i-PrO} & \text{Me} \\ \\ & \text{CF}_3 \end{array}$$

RN 856166-27-3 CAPLUS

CN Benzenepropanoic acid, $4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{CH-CH}_2\text{-CO}_2\text{H} \\ \\ \text{i-PrO} & \text{Me} \\ \\ & \text{CN} \end{array}$$

RN 856166-28-4 CAPLUS

CN Benzenepropanoic acid, β , 3-dimethyl-4-[5-[3-methyl-4-(1-methylethoxy)phenyl]-1, 2, 4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 856166-29-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{i-PrO} \\ \hline \\ \text{Cl} \end{array}$$

RN 856166-32-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-[(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-34-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-35-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(1-pyrrolidinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-36-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(4-morpholiny1)-3-pyridiny1]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-37-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-[methyl(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-38-6 CAPLUS

CN Benzenepropanoic acid, $4-[5-[5-chloro-6-(2,2,2-trifluoroethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

RN 856166-39-7 CAPLUS

CN Benzenepropanoic acid, $4-[5-[5-chloro-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

RN 856166-40-0 CAPLUS

CN Benzenepropanoic acid, $4-[5-[5-chloro-6-(3,3-difluoro-1-piperidinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

RN 856166-41-1 CAPLUS

CN Benzenepropanoic acid, $4-[5-[5-chloro-6-(3,3-difluoro-1-pyrrolidinyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

RN 856166-42-2 CAPLUS

CN Benzenepropanoic acid, β , 3-dimethyl-4-[5-[6-(4-morpholinyl)-5-(trifluoromethyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N} & \text{N} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH} & \text{N} & \text{O} \\ \text{Me} & \text{CF}_3 \end{array}$$

RN 856166-48-8 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-chloro-6-(2-methylpropyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-CH_2-CO_2H \\ \hline \\ i-Bu \\ C1 \end{array}$$

RN 856166-50-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-iodo-6-[methyl(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-51-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-cyano-6-[methyl(1-methylethyl)amino]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-54-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[6-(3,3-difluoro-1-pyrrolidinyl)-5-iodo-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \\ & \text{N} \\ & \text{N} \\ & \text{O} \end{array}$$

RN 856166-55-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[6-(3,3-difluoro-1-pyrrolidinyl)-5-ethynyl-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{C} \\ \text{F} \\ \text{N} \\ \text{O-N} \\ \text{Me} \end{array}$$

RN 856166-74-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-(1,1-difluoro-2-methylpropyl)-2-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-75-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-(5-cyano-6-ethoxy-3-pyridinyl)-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-76-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-cyano-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-77-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-cyano-6-(2-methylpropyl)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-CH_2-CO_2H \\ \hline \\ i-Bu \\ CN \end{array}$$

RN 856166-78-4 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-(1,1-difluoro-2-methylpropyl)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-79-5 CAPLUS

CN Benzenepropanoic acid, 4-[5-[5-iodo-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-80-8 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(cyclopentyloxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$HO_2C-CH_2-CH_2$$
 $N-O$
 $N-O$

RN 856166-81-9 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(2-methylpropoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} \\ \\ \text{i-BuO} \\ \\ \text{Cl} \end{array}$$

RN 856166-82-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CO}_2\text{H} \\ \text{F}_3\text{C}\text{--}\text{CH}\text{--}\text{O} & \text{Me} \\ \end{array}$$

RN 856166-83-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-84-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3,5-dichloro-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{Cl} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2 \\ \hline & \text{N}-\text{O} \end{array}$$

RN 856166-85-3 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-(cyclopropylmethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2 \\ \hline \\ \text{N} \\ \end{array} \begin{array}{c} \text{C1} \\ \text{O}-\text{CH}_2 \\ \hline \end{array}$$

RN 856166-86-4 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-(5-propoxy-2-pyridinyl)-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \\ \text{N} & \text{O--N} \end{array}$$

RN 856166-87-5 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[3-nitro-4-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$MO_2$$
C- CH_2 - CH_2
 NO_2
 O - CH - CF_3
 N
 N
 N
 N
 N
 N

RN 856166-88-6 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{CN} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2 \\ \\ \text{N} \\ \text{O} \end{array}$$

RN 856166-89-7 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-90-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-cyano-4-[(1S)-1-methylpropoxy]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 856166-91-1 CAPLUS

CN Benzenepropanoic acid, 3-methyl-4-[5-[4-(trifluoromethyl)-6-(2,2,2-trifluoro-1-methylethoxy)-3-pyridinyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

RN 856166-92-2 CAPLUS

CN Benzenepropanoic acid, 4-[5-[4-amino-2-(2,2,2-trifluoro-1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

RN 856166-94-4 CAPLUS

CN Benzenepropanoic acid, $4-[5-[3-cyano-4-[(1S)-1-methylpropoxy]phenyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 856166-95-5 CAPLUS

CN Benzenepropanoic acid, $4-[5-[3-cyano-4-[2,2,2-trifluoro-1-(trifluoromethyl)ethoxy]phenyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl-

(CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{CH-CH}_2\text{-CO}_2\text{H} \\ \hline \\ \text{F}_3\text{C-CH-O} & \text{Me} \\ & \text{CN} \end{array}$$

RN 856166-96-6 CAPLUS

CN Benzenepropanoic acid, $4-[5-[3-cyano-4-(2,2,2-trifluoroethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-<math>\beta$,3-dimethyl- (CA INDEX NAME)

RN 856167-09-4 CAPLUS

CN Benzenepropanoic acid, α , α -difluoro- β -hydroxy-3-methyl-4- [5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} \\ \text{CH-CF}_2\text{-CO}_2\text{H} \\ \\ \text{i-PrO} \\ \\ \text{CF}_3 \end{array}$$

RN 856167-14-1 CAPLUS

CN Benzenepropanoic acid, α, α -difluoro-3-methyl-4-[5-[4-(1-methylethoxy)-3-(trifluoromethyl)phenyl]-1,2,4-oxadiazol-3-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CF}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrO} & \text{Me} \\ \hline \\ \text{CF}_3 \end{array}$$

RN 856167-19-6 CAPLUS

CN Benzenepropanoic acid, $4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-\alpha,\beta-dihydroxy-3-methyl-, ($\alpha R, \beta R)$-rel- (CA INDEX NAME)$

Relative stereochemistry.

RN 856167-21-0 CAPLUS

CN Benzenepropanoic acid, $4-[5-[3-cyano-4-(1-methylethoxy)phenyl]-1,2,4-oxadiazol-3-yl]-<math>\alpha$, β -dihydroxy-3-methyl-, $(\alpha R, \beta S)$ -rel- (CA INDEX NAME)

Relative stereochemistry.

RN 856167-30-1 CAPLUS

CN Benzenepropanoic acid, 4-[5-[3-chloro-4-[(1-methylethyl)thio]phenyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2\text{-}\text{CH}_2\text{-}\text{CO}_2\text{H} \\ \hline \text{i-PrS} & \text{Me} \end{array}$$

IT 856166-58-0P, 3-[4-[5-[6-(3,3-Difluoropyrrolidin-1-yl)-5-

[(trimethylsilyl)ethynyl]pyridin-3-yl]-1,2,4-oxadiazol-3-yl]-3-methylphenyl]propanoic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of five-membered heterocycle-substituted benzenepropanoic and related acids as selective S1P1 (EDG1) receptor agonists)

RN 856166-58-0 CAPLUS

CN Benzenepropanoic acid, 4-[5-[6-(3,3-difluoro-1-pyrrolidinyl)-5-[2-(trimethylsilyl)ethynyl]-3-pyridinyl]-1,2,4-oxadiazol-3-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c} \text{C} \\ \text{C} \\ \text{C} \\ \text{SiMe}_3 \\ \text{CH}_2 - \text{CH}_2 - \text{CO}_2 \\ \text{H} \\ \text{O} \\ \text{N} \\ \text{Me} \\ \end{array}$$

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL STNGUIDE COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 32.12 404.10

FULL ESTIMATED COST

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COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.07
404.17

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COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.07 404.17

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STRUCTURE FILE UPDATES: 5 MAY 2009 HIGHEST RN 1143038-16-7 DICTIONARY FILE UPDATES: 5 MAY 2009 HIGHEST RN 1143038-16-7

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=>

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chain nodes :
21 22 23 24 25 27 29 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 26 28 30 31 32 33
34 35 36 37 38 39 40 41 42

```
ring/chain nodes :
18 20
chain bonds :
10 - 12 \quad 15 - 18 \quad 18 - 20 \quad 20 - 21 \quad 22 - 23 \quad 23 - 24 \quad 25 - 26 \quad 27 - 28 \quad 29 - 30 \quad 36 - 43 \quad 40 - 44
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-11 \quad 7-8 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14
14-15 \quad 15-16 \quad 16-17 \quad 26-31 \quad 26-34 \quad 28-35 \quad 28-38 \quad 30-39 \quad 30-42 \quad 31-32 \quad 32-33 \quad 33-34 \quad 33-3
35-36 36-37 37-38 39-40 40-41 41-42
exact/norm bonds :
7-11 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33
33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42
exact bonds :
7-8 8-9 10-12 15-18 18-20 25-26 27-28 29-30
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-17 \quad 22-23
23-24
isolated ring systems :
containing 1 : 7 : 12 :
```

G1:[*1],[*2],[*3],[*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom 29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS 50:Atom

L8 STRUCTURE UPLOADED

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```
chain nodes :
21 22 23 24 25 27 29 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 26 28 30 31 32 33
34 35 36 37 38 39 40 41 42
ring/chain nodes :
18 20
chain bonds :
5-7 10-12 15-18 18-20 20-21 22-23 23-24 25-26 27-28 29-30 36-43 40-44
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14
14-15 15-16 16-17 26-31 26-34 28-35 28-38 30-39 30-42 31-32 32-33 33-34
35-36 36-37 37-38 39-40 40-41
                                   41 - 42
exact/norm bonds :
7-11 8-9 9-10 10-11 20-21 26-31 26-34 28-35 28-38 30-39 30-42 31-32
32-33 33-34 35-36 36-37 36-43 37-38 39-40 40-41 40-44 41-42
exact bonds :
5-7 7-8 10-12 15-18 18-20 25-26 27-28 29-30
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-17 \quad 22-23
23-24
isolated ring systems :
containing 1:7:12:
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:CLASS 28:Atom 29:CLASS 30:Atom 31:Atom 32:Atom 33:Atom 33:Atom 33:Atom 33:Atom 37:Atom

38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:CLASS 44:CLASS

G1:[*1],[*2],[*3],[*4]

Match level :

L9 STRUCTURE UPLOADED

=> s 18 sss full

FULL SEARCH INITIATED 20:39:02 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L10 0 SEA SSS FUL L8

=> s 19 sss full

FULL SEARCH INITIATED 20:39:07 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 25 TO ITERATE

100.0% PROCESSED 25 ITERATIONS 5 ANSWERS

SEARCH TIME: 00.00.01

L11 5 SEA SSS FUL L9

=> file capl

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E FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 371.28 775.45

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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

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L12 0 L11